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Full Length Research Paper

Application of nonlinear reduction techniques in chemical process modeling

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Model reduction techniques have been used widely in all engineering fields especially in electrical, mechanical as well as chemical engineering. The basic idea of reduction technique is to replace the original system with much smaller state space dimension. A reduced order model is more beneficial to process and industrial field in terms of control purposes by using proper orthogonal decomposition method (POD), which finds applications in computationally processing large amounts of high-dimensional data with the aim of obtaining low-dimensional descriptions that capture a large amount of the phenomena of interest. The discrete version of the POD, which is the singular value decomposition (SVD) of matrices, is described in some detail.

Key words: Model reduction technique, nonlinear model, proper orthogonal decomposition.

INTRODUCTION

The developments of mathematical models are based on: (i) theoretical models using the principles of chemistry and physics, (ii) empirical models, obtained from the statistical analysis of the operating data's process and (iii) semi empirical hybrid models. The issue of development of the nonlinear process model is very important and is more challenging in an industrial setting. The fundamental models have several advantages over the other models, for example, it requires less process data, the model parameters can be estimated from laboratory experiments and routine operating data instead of time consuming plant test, and it can be extrapolated to operate on regions which are not represented in the data set used for model development (Henson, 1998).

The major drawback of the fundamental dynamic model is the highly nonlinear state dimension of the system and its complexity too. Thus, the models are not well suited for incorporation into the control scheme. Moreover, the derivation of dynamic models for large scale process is difficult.

Modeling is a common theme within the simulation, control and optimization of processes. However, model reduction techniques have become more popular. The aim of almost any reduction technique is to provide a reduced order model that can be used for controller design.

There are two approaches to reduce the model (Johan et al., 2005):

1. Reducing the system with respect to the physics of the system.
2. Project the system onto smaller subspace.

The concept of the first approach will be better if we have good knowledge regarding the system. However, the drawback is that this approach can not be used to black box the model because they have different techniques for each system. The second approach has a disadvantage which is, the reduced system is not as good as expected for a physical meaning anymore. The limits of applicability of these techniques are represented by a big difference between the real and theoretical systems. Also, reducing the effects of inputs parameters inside the system does not lead to a clearer view about the real system.

In this paper, we will focus on a proper orthogonal decomposition (POD) method that reduced the nonlinearity of the system.

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Lall et al. (1999) have developed a method of model reduction for the nonlinear system. The method requires only standard matrix computations for the used balanced truncation in the linear system. For the nonlinear system, the method is used for the POD.

Hahn and Edger (2002) have improved the technique by Lall et al. (1999) which reduced the nonlinear system especially for the ordinary differential equation system. The proposed technique is a balancing technique used for POD and Galerkin projection.

Hedengren and Edger (2005) have developed the adaptive order reduction of large scale nonlinear differential algebraic. This method includes three steps: adaptive with POD, algebraic state and *in situ* adaptive tabulation which is used to transform the implicit sets into linear explicate approximation.

Sun and Hahn (2005) have implemented a reduction technique on stable nonlinear differential algebraic equation systems. This method (POD) reduces the other differential equations for a model of distillation column as a case study.

The POD has been used to obtain approximately, low-dimensional descriptions of turbulent fluid flows (Holmes et al., 1996), structural vibrations (Cusumano et al., 1994) and insect gait, and has been used for damage detection to name a few applications in dynamic systems. Also, it has been extensively used in image processing, signal analysis and data compression.

METHODOLOGY

Suppose we wish to approximate a function of z(x, t) over some domain of interest as a finite sum in the variables separated form:

$$z(x,t) = \sum_{k=1}^{M} a_k(t)k(x) \qquad (1)$$

It is reasonably expected that the approximation becomes exact in the limit as M approaches infinity, except possibly on a set of measure zero (readers unfamiliar with the measure theory may ignore it if they deal with finite-dimensional calculations; and consult, for example, Rudin 9 otherwise).

While in Equation (1) there is no fundamental difference between t and x, we usually think of x as a spatial coordinate (possibly vector-valued) and t as a temporal coordinate. Thus, the representation of Equation (1) is not unique. For example, if the domain of x is a bounded interval of x on the real line, then the functions of f k(x) can be chosen as either a Fourier series, Legendre polynomials, Chebyshev polynomials, and so on. For each, such choice of a sequence of f k(x) that forms a basis for some suitable class of functions z(x, t) and the sequence of time-functions ak(t) is different. That is, for sines and cosines we get one sequence of functions for ak(t), while for Legendre polynomials we get another, and so on. The POD is concerned with one possible choice of the functions of f k(x). However, if we have chosen the orthonormal basis functions, we will have:

$$\int_x k_1(x)k_2(x)dx = \begin{cases} 1 \ if \ k_1 = k_2 \\ 0 \ otherwise \end{cases} \qquad (2)$$

$$a_k(t) - \int_x z(x,t)k_x d(x)$$

For the orthonormal basis functions, the determination of the coefficient function of ak(t) depends only on f k(x) and not on the other f 's. What criteria should we use for selecting the functions of f k?

Orthonormality would be useful; moreover, while an approximation to any desired accuracy in Equation (1) can always be obtained if M can be chosen adequately, we may likely choose the f k(x) in such a way that the approximation for each M is as good as possible in a least squares sense. That is, we would try to find, permanently, a sequence of orthonormal functions f k(x) such that the first two of these functions give the best possible two-term approximation, the first seven give the best possible seven term approximation, and so on. These special, ordered, orthonormal functions are called the proper orthogonal nodes for the function of z(x, t). Nonetheless, orthonormality would be the expression that is called the POD of z(x, t) in Equation (1).

Mathematical expression

Consider a system where measurements of m state variables are taken (these could be from m strain gauges on a structure, or m velocity probes in a fluid, or a mixture of two kinds of probes in a system with flow-induced vibrations, etc.), and assume that at N instants of time, measurements of N sets of m are taken simultaneously at these m locations. We arrange the data in an N × m matrix A, such that element Aij is the measurement from the jth probe taken at the ith time instant. The m state variables are not assumed to be measured by transducers that are arranged in some straight line in the physical space. We merely assume that the transducers have been numbered for identification, and that their outputs have been placed side by side in matrix A. In the actual physical system, these measurements might represent one spatial dimension (for example,

accelerometers on a beam), or more than one spatial dimension (for example, pressure probes in a three dimensional fluid flow experiment). Each physical transducer may itself measure more than one scalar quantity (for example, triaxial accelerometers). In such cases, the different scalar time series from the same physical transducer are arranged in different columns of A. Here, the final result of the data collection is assumed to be the N × m matrix A.

It is common to subtract, from each column of A, the mean value of that column. Whether or not this is done does not affect the basic calculation, though it affects the interpretation of the results.

Notwithstanding the previous warnings, through a combination of engineering judgement and luck, the POD continues to be fruitfully applied in a variety of engineering and scientific fields. Judging from the study, it is a useful tool at least for people who regularly deal with moderate to high dimensional data.

The singular value decomposition

We now compute the singular value decomposition (SVD) of matrix A, which is of the form (Joan et al., 2006):

$$A = U\Sigma V^T \quad (3)$$

where U is an N × N orthogonal matrix, V is an m × m orthogonal matrix, the superscript T indicates matrix transpose, and Σ is an N × m matrix with all its elements equal to zero, except along the diagonal. The diagonal elements of Sii consist of r = min (N, m) and nonnegative numbers of si, which are arranged in decreasing order, that is, r ≥ 0. The s's are called the singular values of A (and also of A^T) and are unique. The rank of A equals the number of nonzero singular values. In the presence of noise, the number of singular values which is larger than some suitably small fraction of the largest singular value might be taken as the 'numerical rank'. Since the singular values are arranged in a specific order, the index k of the kth singular value will be called the singular value number as shown in Figure 1.

Correspondence with Equations (1) and (2): In Equation (3), let US = Q. Then the matrix Q is N × m, and $A = QV^T$. Letting qk be the kth column of Q and v_k the kth column of V, we write out the matrix product as:

$$A = QV^T = \sum_{k=1}^{M} q_k \quad v_k^T \quad (4)$$

Equation (4) is the discrete form of Equation (1). The function of z(x, t) is represented here by matrix A. The function of ak(t) is represented by the column matrix qk, while the function of f k(x) is represented by the row matrix v_k^T. The approximation of Equation (1) is now exact because the dimension is finite. Due to the orthonormality of the columns of V, Equation (2) corresponds to the multiplication of Equation (4) by one of the V's on the right.

Relationship between temperature, distance and time represents a suitable example of the high nonlinearity system as shown in Equation (5):

$$T(x,t) = \exp^{-(x-0.5)(t-1)} + \sin(x,t), \quad 0 \le x \le 1,\ 0 \le t \le 2 \quad (5)$$

Imagine that we 'measure' this function at 25 equally spaced x points, and 50 equally spaced instants of t. The temperature of z(x, t) is shown in Figure 1a. Arranging the data in matrix Z, we compute the SVD of Z, and then compute rank 1, rank 2 and rank 3 approximations to Z, as shown in Figure 1. MATLAB software is used for Equation (5) to reduce the order by calculating the SVD and POD as shown in Figure 1. The rank 3 approximation (Figure 1) looks indistinguishable from the actual temperature as shown in Figures 1 and 2. This is explained by Figure 1 which shows the singular values of Z. Note how the singular values decrease rapidly in magnitude, with the fourth one significantly smaller than the third (The numerical values are 47.5653, 2.0633, 2.0256, 0.0413, 0.0106 . . .).

Note that in this example without noise, the computed singular values beyond number 14 flatten out at the numerical roundoff floor around 10 to 15. The actual singular values beyond number 14 should be smaller, and an identical computation with more digests of precision should show the computed singular values flattening out at a smaller magnitude. Conversely, perturbing the data matrix by zero mean random numbers of typical magnitudes, 10 to 8 causes the graph of singular values to develop an obvious elbow at about that value. For experimental data with noise, the SVD of the data matrix can sometimes provide an empirical estimate of where the noise floor is. So far in this example, we have merely computed the lower rank approximations to the data, and the use of the SVD in the calculation may be considered incidental. Now, suppose we wish to interpret the results in terms of mode shapes, that is, in the context of the POD, the first 3 columns of V provide the 3 dominant x-direction mode shapes, and on projecting the data onto these mode shapes we can obtain the time histories of the corresponding modal 'coordinates'. The calculation of the modal coordinates is straightforward. Using Equation (4), t he kth modal

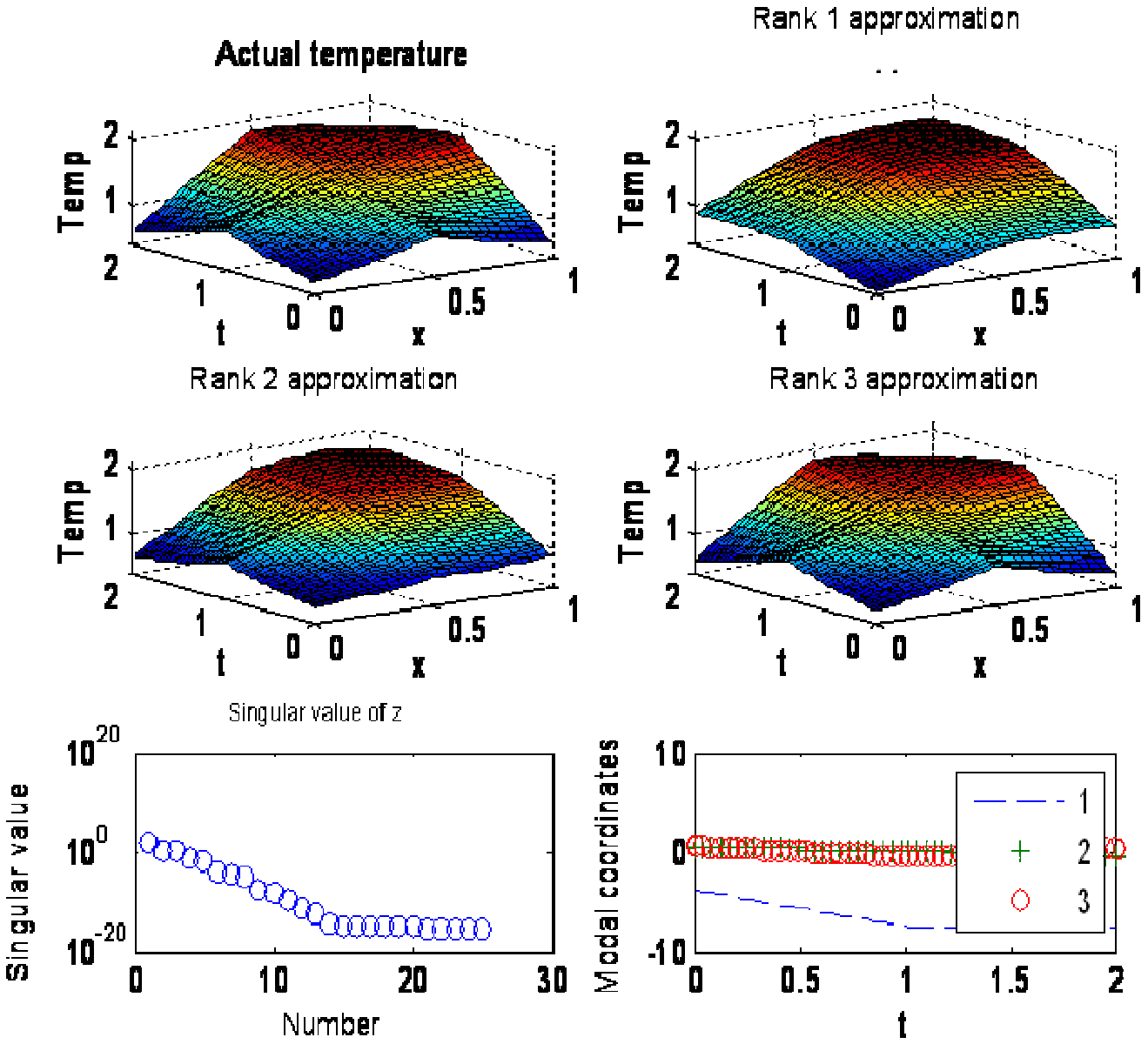

Figure 1. Approximation of temperature.

coordinate of q_k is simply uksk, where uk is the kth column of U (assuming U is available from the SVD). Alternatively, if only the proper orthogonal modes of V are available, then the projection calculation is simply $q_k = Av_k$, where v_k is the kth column of V. The modal coordinates for the temperature given by Equation (5) are plotted in Figure 1. The first coordinate is obviously dominant (the first singular value is dominant), while the second and third have comparable magnitude (singular values 2 and 3 are approximately equal) as shown in Figure 2. Rank 3 is the best because the difference between the actual value and approximation valuesfor Ranks 1, 2 and 3 gave high approximation for rank 3 which reaches 97.34% as shown in Figure 2.

Consider the differences between the SVD and eigenvalue decomposition. The SVD can be computed for non-square matrices, while the eigenvalue decomposition is only defined for square matrices. The SVD remains within the real arithmetic whenever A is real, while eigenvalues and eigenvectors of unsymmetric real matrices can be complex. Each of the left and right singular vectors (columns of U and V, respectively) is orthogonal, while eigenvectors of unsymmetric matrices need not be orthogonal even when a full set exists. Finally, while an eigenvector (say) ψ and its image A ψ are in the same direction, a right-singular vector v_k (kth

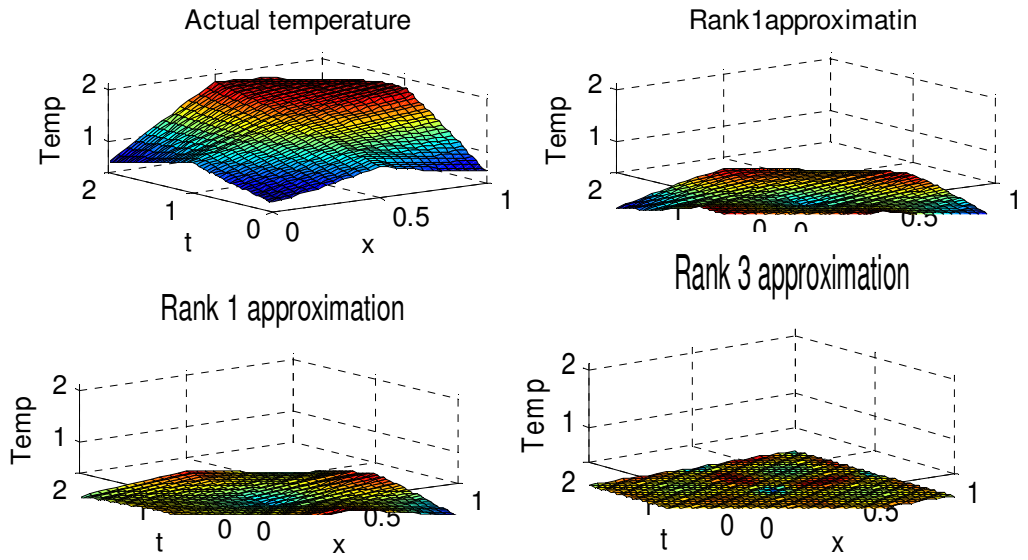

Figure 2. Difference between actual and rank approximation methods.

column of V) and its image Av_k need not be in the same direction or even in spaces of the same dimension. However, the SVD does have strong connections with the eigenvalue decomposition. On premultiplying Equation (3) with its transpose and noting that $V^{-1} = V^T$, we see that V is the matrix of eigenvectors of the symmetric m × m A^T A matrix A^T A, while the squares of the singular values are the r = min (N, m) largest eigenvalues of A^T A.

CONCLUSIONS

A few reduction techniques applied in the chemical process have been reviewed. It was found that the number of reduced techniques application in the chemical processes was still low. However, POD represented one of the important methods that can be used to reduce the nonlinearity of the system without having high effects on the behavior of the system.

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